

Computer Simulation Center in Internet

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Abstract: The general description of infrastructure and content of SciShop.ru computer simulation center is given. This resource is a new form of knowledge generation and remote education using modern Cloud Computing technologies.

Keywords: Cloud computing, internet, information technologies, computer simulation, program complexes, remote access, remote education.

1 Introduction

Recent achievements in the area of information technologies and Internet give the reasons to believe that the new methods of the organization of the scientific knowledge exchange process have already been formed by now, and in the near future, one may expect a general passage from the conventional techniques of the scientific knowledge dissemination via the paper journals to their electronic counterparts.

The present paper is devoted to one of the advanced aspects of the scientific knowledge dissemination – a new form of the transfer of the developed intellectual product, the program complexes for solving various scientific and applied problems from the developers to the users.

The process of the transfer of computational complexes conventionally consisted of the fact that the consumer (the future user) acquired the codes (in some cases also the program texts) from the code developers and then installed them on his computer. To ensure a reliable and declared work of the program complex the user must have a similar operation medium, including the systems for visualizing the digital data.

The stage of the installation of computer programs is, on the whole, very complex even when a support by the developer is provided, and it often causes many difficulties the surmounting of which requires considerable, intrinsically non-productive expenses of intellectual efforts and time.

The new form of using the computational complexes frees from all problems related to the installation of the acquired program product.

A special site – the Computer Simulation Center – is created in the Internet. This Center hosts the program complexes with all their attributes: the preprocessor system for preparing the tasks, the processor system for executing the tasks (executing the computational operations), and the postprocessor system for the output of the obtained information in the digital and graphical forms.

The user must only formulate his own computational task by performing the input of numerical data and starting its numerical solution. He will be provided with the solution of his task upon the

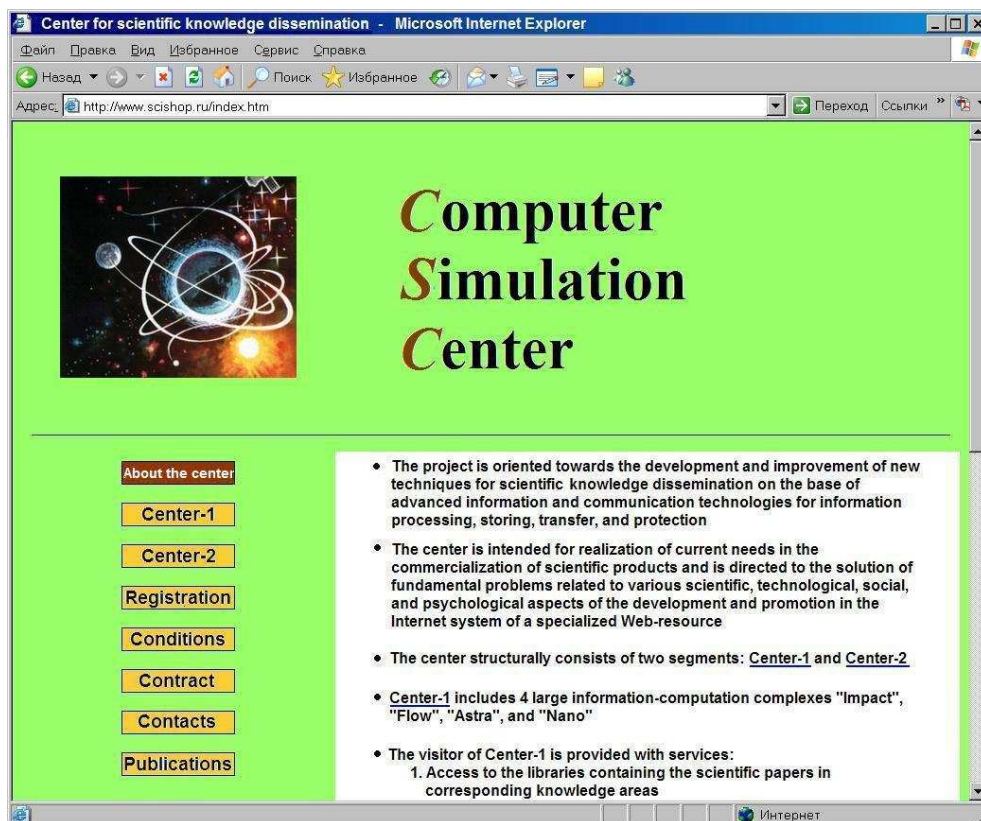


Figure 1: Main page of the Computer Simulation Center in Internet (a fragment).

termination of computations. Special services of the client's support must provide a comfort of the visitor's stay at the Center. In the economic terms, such a method of using the program complexes means their leasing from the resource developers.

The Computer Simulation Center SciShop.ru is a pioneer of this new direction of the development of the advanced information technologies. The Center was created as a result of the execution of the series of works (see, for example, [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]).

A general description and the infrastructure of the Center are presented in [1, 2, 3], and its content, the information-computational complexes for solving the tasks from a number of scientific areas are presented in [4, 5, 6, 7, 8]. At present, the Computer Simulation Center is functioning successfully in the Worldwide web and is subject to its continuous modernization and development (see [10, 11]).

This project is directed to the application of breakthrough technologies in the domain of the development and improvement of new techniques for scientific knowledge dissemination with the use of the Worldwide web and is intended for a remote teaching of the specialists, postgraduates, and students to the methods of mathematical modelling and practical training in the solution of scientific and applied problems. The teaching and training are carried out on the basis of efficiently functioning program complexes whose composition is continuously enriched.

2 Computer Simulation Center SciShop.ru

The project on the development of the Computer Simulation Center ([http://www. SciShop.ru](http://www.SciShop.ru)) is oriented towards the development and improvement of new techniques for scientific knowledge dissemination on the basis of the advanced info-communication technologies for the information processing, storing, transfer, and protection.

- The Center is intended for the realization of current needs in the commercialization of scientific products and is directed to the solution of fundamental problems related to various scientific, technological, social and psychological aspects of the development and promotion in the system of the specialized Internet Web resource.

- The Center structurally consists of two segments: Center-1 and Center-2.

- Center-1 includes four large information-computational complexes “Shock”, “Flow”, “Astra”, and “Nano”.

- The following services are provided for the visitor of Center-1:

1. The access to the libraries containing the scientific articles in corresponding knowledge areas.
2. The access to tabular and/or graphical databases containing the results of computer simulation of the corresponding computer tasks.

3. The access to processor systems enabling for the client himself the organization and execution of computer simulation of the problems, which are of interest to him.

4. The access to the locks to pass to the sites of the leading Russian and foreign journals in corresponding knowledge areas.

5. The access to the segment “Forum” for obtaining the consultations and discussion of problems.

- In the non-commercial regime, the visitor has the access to the demo versions of the systems of Center-1. For a full-scale access, one should register and perform the payment.

- The system of the Center for accepting the payments accepts the payment from any electronic payment systems (WebMoney, Yandex.Money, E-gold, etc., which enter the Robokassa consortium). The system for accepting payment with the use of the bank credit cards and SMS messages of the cellular communications has been developed and is now under verification.

- Center-2 is intended for positioning the program developments in various branches of knowledge without any limitations for the themes. The content of this section may be augmented by the resources of any specialists having the copyright for these information resources.

- All the specialists in the field of computer simulation in any knowledge areas, which have the program developments and wish to promote them, also on the onerous basis, are invited for a cooperation with Center-2. The specialists wishing to place their scientific products at Center-2 should familiarize themselves with the conditions of their placement, get in touch with the administration of the Center, and to sign a Contract.

- One can familiarize himself in detail with all aspects of the Center functioning in the special section “Publications” by using the corresponding hyperlink on the site Main page (Fig. 1).

3 General characteristic of the arrangement of computations at the center and the advantages of the direct computer simulation in Internet

The comfort of the client’s stay in the Internet center and a convenient form of using its segments: the bibliographic section, databases containing already obtained tabular and graphical information, and especially the processor systems are the most important attributes of any program complex. Right this is usually most difficult for the user.

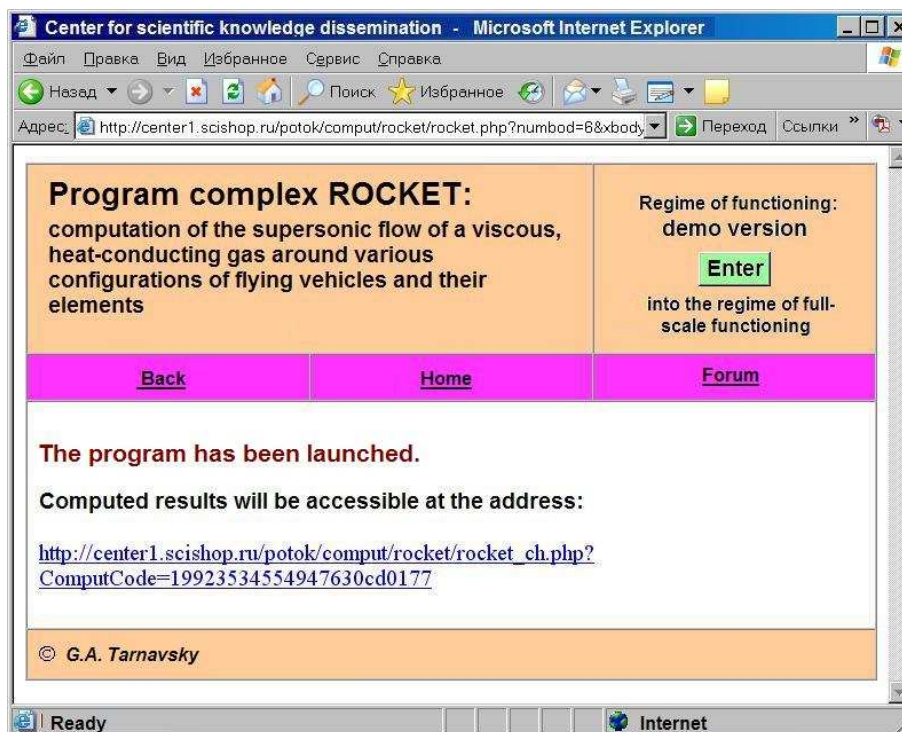


Figure 2: Site page with the messages for the client that the computation of the task formed by him has been launched, and its solution will be accessible at the indicated URL address.

The systems for the pre-processor preparation of tasks (the input of parameters and the start-up of processor systems) are arranged in a clear, convenient, and simplest form, which eliminates an ambiguous interpretation and difficulties for the specialists having even a small experience.

The operations with the processor systems are carried out by the user in the regime of remote access in the Worldwide web on its local portal – directly at the computer simulation center rather than on its own computer after the installation of the complex. This gives for the visitor of the Center a possibility to carry out the study of the computational complex, to organize the solution of the problem of interest, and to obtain the results of computer studies.

The transfer of a computational complex usually consists of the purchase of the license, documentation, and computer codes. After that, the user performs the installation of the purchased product on its own computer facility. As a rule, this occurs with large difficulties, which may be due to various reasons, from using different versions of the operating system to the peculiarities of the supporting systems installed on computers of the seller and the purchaser.

There are no such problems when the processor systems are placed at the Center. All the interfaces have been debugged, well tested and adjusted. The functioning of complexes is faultless in the specified ranges of parameters variation (note that one can always ask any question on the site forum and obtain the explanation). The fact that the user is freed from the necessity of buying the hardware (which is often very costly) necessary for performing the needed computations is one more advantage of this approach. The user in fact “leases” the hardware from the site developers only for the time of the solution of his task.

We emphasize that such an efficient method of using the processor complexes by the visitors of the Center has required the development and implementation of original solutions. Since neither of

the Internet providers will permit the execution of many and, possibly, long-term computations on his node, which would take many resources and reduce the capacity of channels, one would need the use of a different scheme for execution of computations.

The client organizes at the Center his computational task (chooses the processor system and inputs the parameters in it) and starts up the computation on the system. The systems of this site segment on the support of tasks pack the task into a file and send it via the net to the computing center containing a number of computers, including the multi-processor systems. The task is solved here, the results (Fig. 2) are forwarded either to the Center, if the client waits for them, or to its home address in the net. This scheme has shown itself very well during its beta testing.

4 The system for registering clients and commercial system of the center

The program complexes of the Center may be used both free of charge (the demo versions) and on a commercial basis. The access to the regime of the full-scale functioning of the center is realized after the visitor registration in the specialized "book of record" (Fig. 3) and after the visitor transfers the user charge via the electronic payment systems.

The use of the specialized bank system "Robokassa" has been organized (together with the development of necessary interfaces) for the commercial segment of the center. This system enables the use of more than 20 electronic payment systems (WebMoney, Yandex.Money, Internet.Money, Internet.Groschi) as well as a number of foreign electronic payment systems of the type E-Gold, PayPal, MoneyBookers, EuroCash, etc. for the purpose of a significant broadening of the scope of clients. A system has also been implemented, which makes it possible to carry out the payments by using the SMS cellular communications (Fig. 4). The safety of the passage of payments, the transparency of their routing, the necessary messages for the client, the currency conversion in different electronic payment systems are guaranteed by special structures of the "Robokassa" system and have been checked in the course of the beta testing of the Computer simulation center.

One should, however, emphasize that the profit earning is not set at present as a predominant goal of the present many-sided project, which is a functional study of the problems of the scientific knowledge dissemination based on advanced information technologies.

5 The center content

The site SciShop.ru is a developing Center of computer simulation. At present, it contains four working information-computation complexes (ICCs):

- "Shock", the high-velocity internal aerodynamics: the computation of shock-wave structures at the inlet to the diffuser of a hypersonic scramjet engine;
- "Flow", the high-velocity external aerodynamics: the computation of the flow around the objects in the atmospheres of the Earth and Mars;
- "Astra", the computational astrophysics: simulation of the dynamics of processes in the intergalactic gas and protoplanet clouds;
- "Nano", microelectronics: computer support of the design of nano-structured semiconductor materials.

Each of these complexes includes the bibliographic section, tabular and graphical databases, which contain the results of the computation of problems in their subject areas as well as the processor systems, which enable the visitor to organize independently the solution of the task of interest. All the resources were created and improved in the course of the execution of numerous computational experiments.

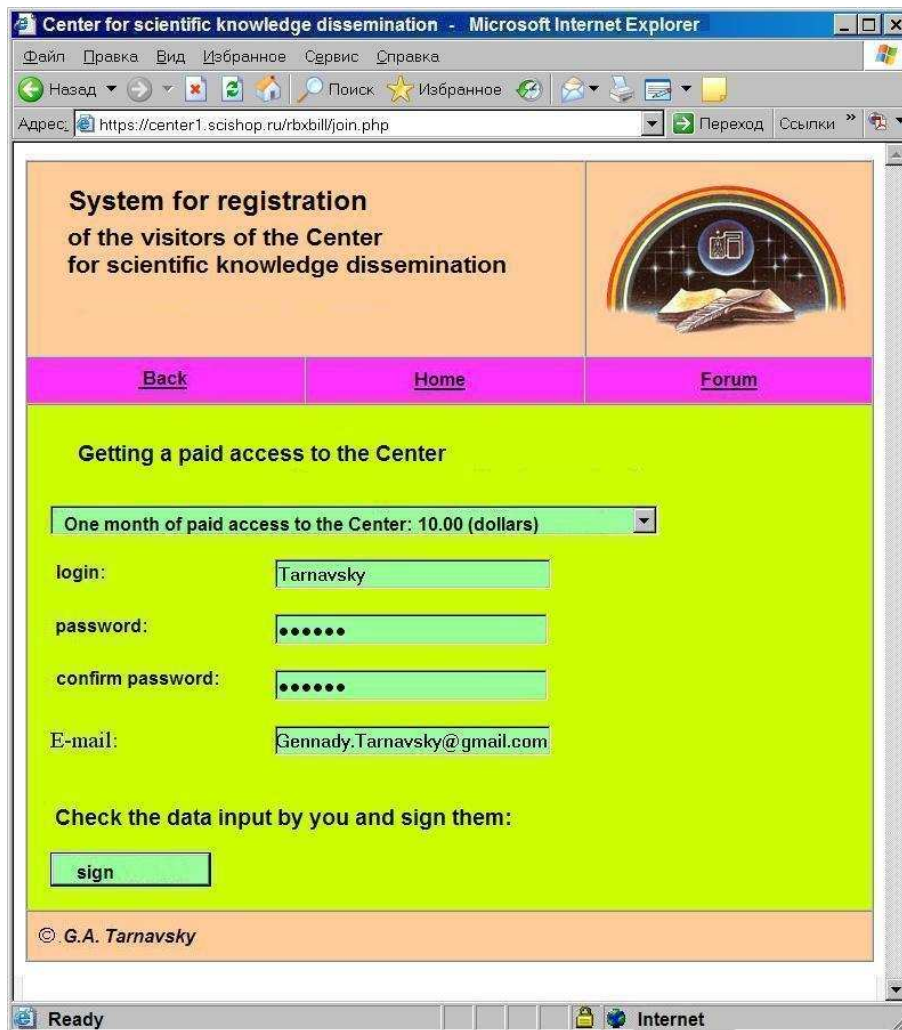


Figure 3: Base page of the site section “The system for registration of the visitors of the Computer Simulation Center”.

ICC “Shock” (Fig. 5). A wide spectrum of the investigations of the shockwave flow patterns arising at the hypersonic scramjet engine inlet was done in the works [3, 4] with regard for the variation of the gaseous medium properties on shocks. The configuration of shocks, the type of their interaction (the Mach and/or regular type) and the flow parameters between the shock fronts under the variation of the flight altitude in the Earth atmosphere from 0 to 100 km, the flight velocities from 1.5 to 7 km/s, the diffuser angles from 0 to 50 degrees were determined.

ICC “Flow” (Fig. 6). The investigation of steady and unsteady flows of both ideal gas (the model of Euler equations) and viscous, heat-conducting gas (the model of full Navier–Stokes equations) around the bodies of different configurations was carried out in the works [5, 6] on the basis of specially developed methods and numerical algorithms within a wide range of determining parameters. The flow structures near the forebody, above the body lateral surface and the body base as well as the flows in the near and far wake of the body were investigated. The characteristic and peculiarities of these structures were determined depending on flight regimes, including the case of

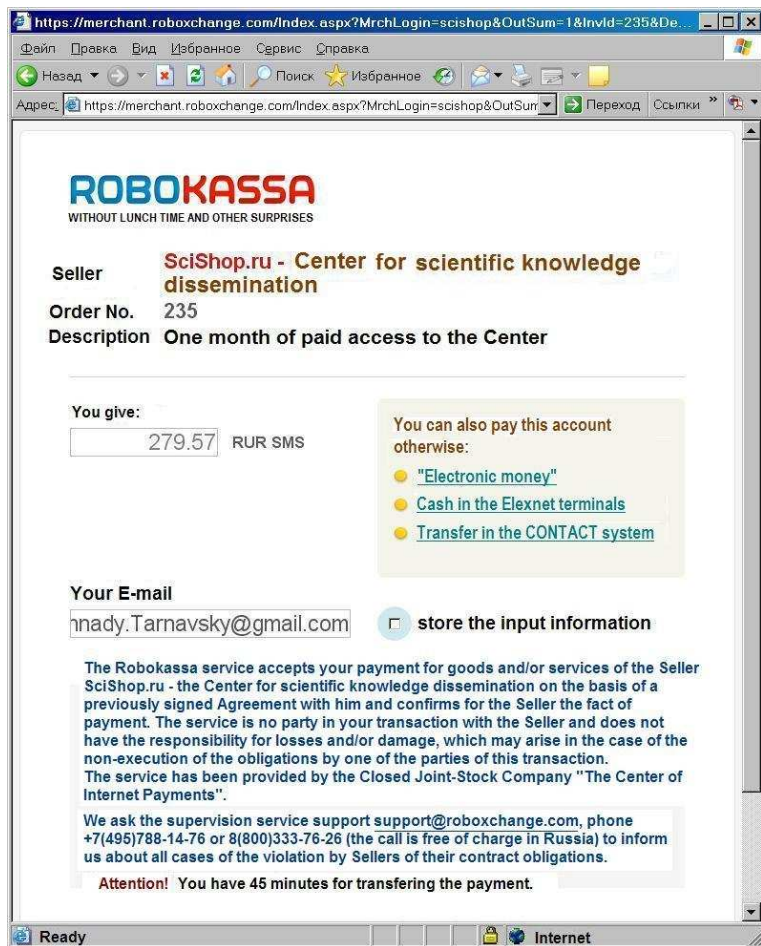


Figure 4: One of the pages of the site section “Transfer of user charge via the SMS messages of cellular communications”.

a localized energy supply to the free stream with the formation of a complex flow pattern of the arising internal shock waves, which are determined by the frequency of the sequence of external source pulses, which may lead to resonance phenomena when an insignificant power of pulses gives rise to a substantial destabilization of the flow, high force and thermal loads on the body surface.

The complex enables the modelling of the aerodynamics of the supersonic and hypersonic flight in the Earth's atmosphere at the altitudes from 0 to 100 km within the speed range from 0.8 to 10 km/s as well as, to a certain accuracy (in accordance with available data), a high-velocity flight in the Mars' atmosphere.

In these works, the most important problems of the adequacy of the mathematical model and the algorithms and codes realizing it to the occurring physical process were studied at a qualitatively new level. Three segments of this question, which are related to the nonuniqueness, were considered: the analytic solutions of the Euler equations, numerical solutions of the full Navier–Stokes equations, and the symmetry loss in symmetric problems. The processes of the evolution of the pattern of the flow around the body with the possibility of a passage from one solution branch to another were studied, and the attraction basins of solutions were determined. The trajectories of the computation motion from the starting solution to the final (steady, quasi-steady, unsteady aperiodic) solution in

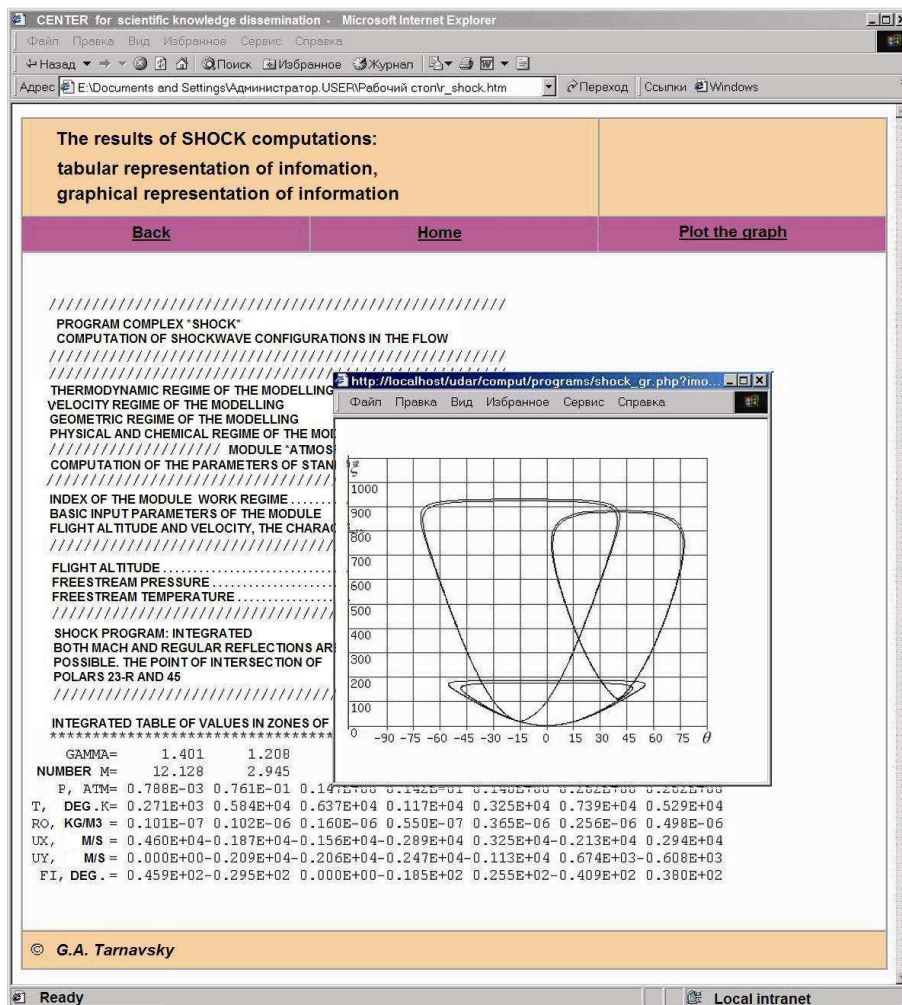


Figure 5: Information-computation complex "Shock". Tabular-digital and graphical representation of the results.

the space of solutions were studied.

ICC "Astra" (Fig. 7). The physical, mathematical, and computational problems of modelling the unsteady three-dimensional problems of the extraterrestrial gas dynamics were considered and analyzed in the work [7]. The system of the Euler gas dynamic equations, which was completed by the force and energy components to model the deviation of the equation of state from the ideal one, the heat-transfer processes (heat conduction, convection, and radiation), gravitation (the gravity field of the point mass and the self-gravitation of a distributed gaseous cloud), was used as the governing system of the differential equations of the mathematical model. The modelling was carried out on the basis of the principle of the decomposition of the complete problem into several sub-problems corresponding to different physical processes. The structuring of the computational complex into several autonomous segments, in its turn, corresponded to this decomposition. This ensures the possibility for extension and supplement of the package of computer programs. The series of the computations of problems on the motion of shock waves and expansion waves in intergalactic gaseous media, on the gravitational collapse of motionless and rotating gaseous clouds, the recession of a

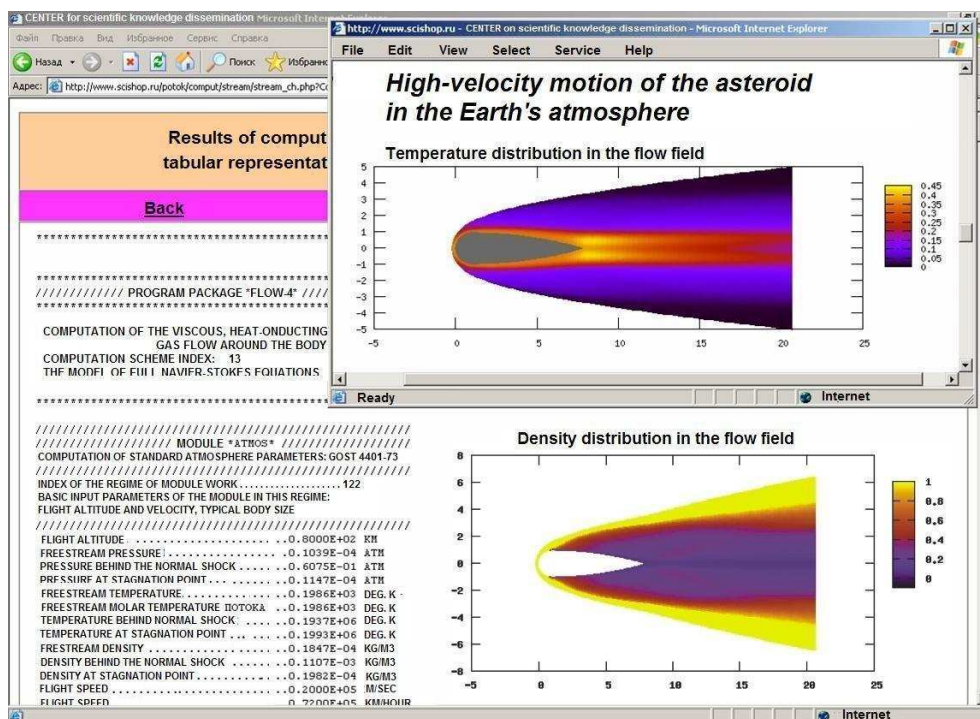


Figure 6: Information-computation complex “Flow”. Tabular-digital and graphical representation of the results.

gaseous cluster, which model the formation and explosion of proto-stars, were done. A thorough verification of the theoretical method, the computational algorithm, and complex of computer codes was done for a comprehensive analysis of their properties (the accuracy of computation and the speed of the computational process).

ICC “Nano” (Fig. 8). Theoretical methods were developed in the work [8] for mathematical modelling of a number of physical-chemical and mechanical processes of the technological cycle of the production of new semiconductor materials, in particular, the motion of the oxidation wave in silicon, including the case of the availability of technological masks ensuring special configurations of the interfaces “material/oxide” with the formation of multiply connected regions. These methods were the basis for developing the efficient numerical algorithms and the complex of computer programs.

Special methods, high-accuracy algorithms, and computer codes were developed for computing the physical processes of the segregation of dopant donor and acceptor admixtures (boron, antimony, and arsenic) at the oxidation wave front in a free-crystalline and prestressed silicon [9].

The computer simulation of the formation of specific nanostructures – narrow localized zones of an elevated electric conductivity of the n- and p-types was conducted.

The complex enables the design of nano- and microelectromechanical systems (diodes, capacitors, transistors, etc.) entering the large, very large, and ultra large integral circuits.

A many-sided experience obtained in the course of the works was implemented in the algorithms of program complexes, which are granted to the visitors of the Center [10, 11] for solving their own tasks in the corresponding knowledge areas.

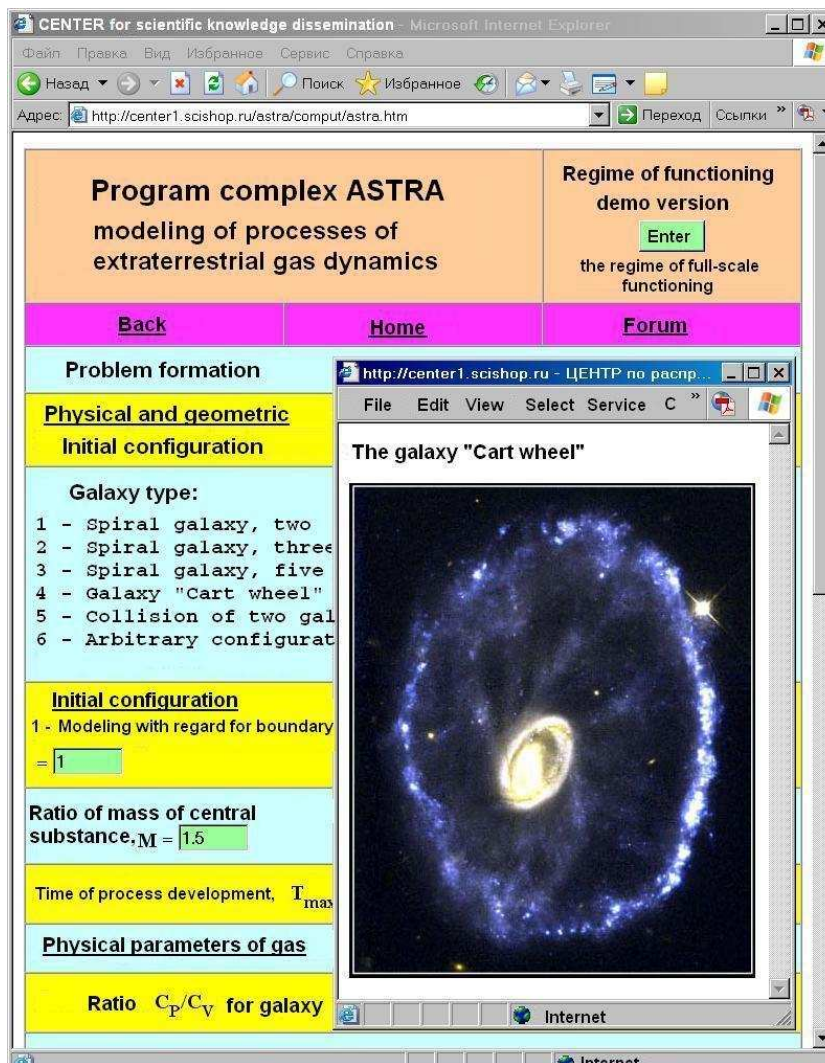


Figure 7: Information-computation complex “Astra”. Page for the preparation of tasks and graphical representation of the results.

6 Conclusion

The infrastructure and content of the Computer simulation center SciShop.ru, the pioneer of a new form of the scientific knowledge dissemination, were briefly considered in the present paper. This center is intended for a direct use of program complexes for the mathematical simulation of processes in various scientific areas, and it provides the possibility of a direct execution of computations in Internet in the remote access regime. Such a form has wide prospects of the application in scientific research and applied developments as well as for a remote teaching of specialists, postgraduates, and students.

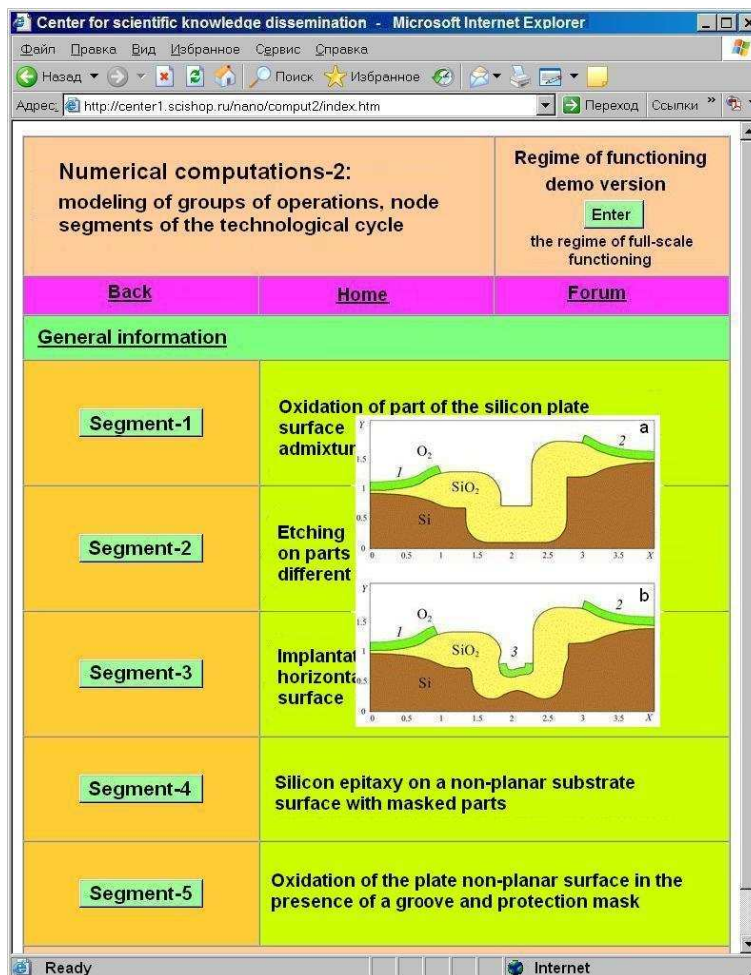


Figure 8: Information-computation complex “Nano”. The page of a task for simulation of the groups of technological operations and graphical representation of the results.

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